



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 03:56 PM EST

PDB ID : 7LMC  
Title : Structure of SARS CoV-2 main protease shows simultaneous processing of its N- and C-terminii  
Authors : Gajiwala, K.S.; Ferre, R.A.; Liu, W.; Ryan, K.  
Deposited on : 2021-02-05  
Resolution : 2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

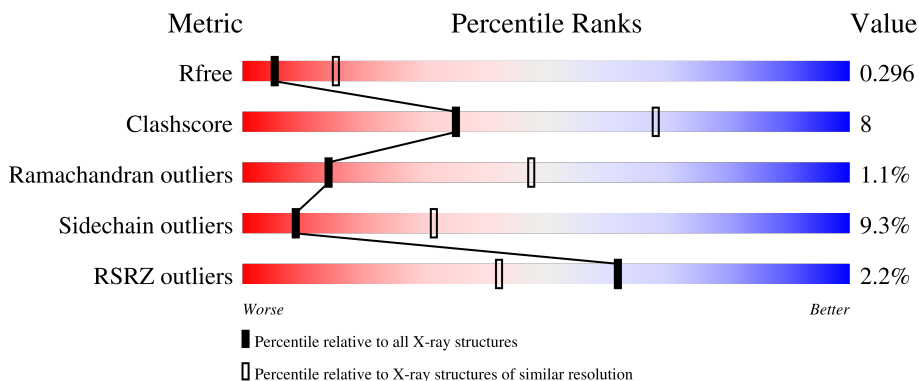
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	6	67% 33%
1	F	6	17% 50% 33% 17%
2	A	306	% 81% 17% .
2	B	306	% 74% 25% .
2	C	306	4% 71% 28% .

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Mol	Chain	Length	Quality of chain
2	D	306	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '3%', a large green segment in the middle labeled '70%', and a yellow segment on the right labeled '27%'. A small black dot is visible at the far right end of the bar.</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9539 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Non-structural protein 4 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	E	6	42	26	7	9	0	0	0
1	F	6	42	26	7	9	0	0	0

- Molecule 2 is a protein called 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	306	2366	1499	402	444	21	0	0	0
2	B	306	2366	1499	402	444	21	0	0	0
2	C	306	2366	1499	402	444	21	0	0	0
2	D	305	2357	1494	400	442	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ALA	CYS	engineered mutation	UNP P0DTD1
B	145	ALA	CYS	engineered mutation	UNP P0DTD1
C	145	ALA	CYS	engineered mutation	UNP P0DTD1
D	145	ALA	CYS	engineered mutation	UNP P0DTD1

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Non-structural protein 4 peptide

Chain E: 




- Molecule 1: Non-structural protein 4 peptide

Chain F: 




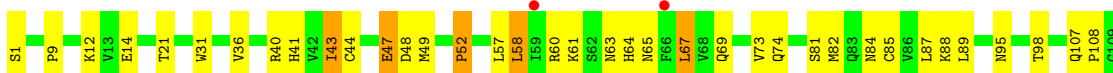
- Molecule 2: 3C-like proteinase

Chain A: 

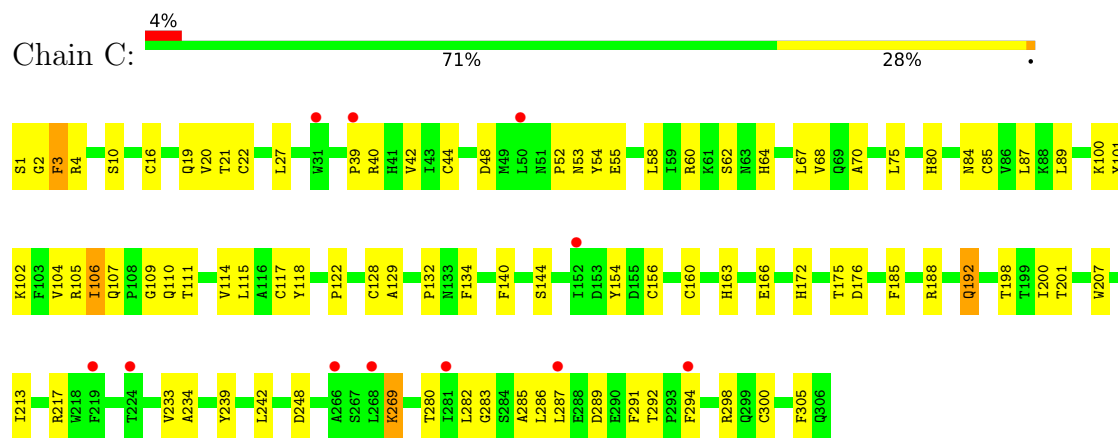


- Molecule 2: 3C-like proteinase

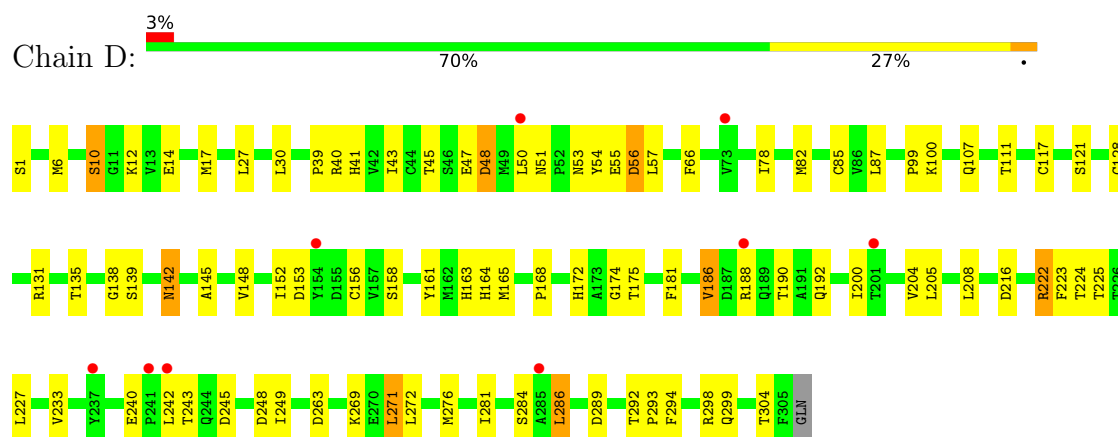
Chain B: 



- Molecule 2: 3C-like proteinase



- Molecule 2: 3C-like proteinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.77Å 66.30Å 80.26Å 80.52° 89.46° 70.55°	Depositor
Resolution (Å)	79.07 – 2.98 79.07 – 2.98	Depositor EDS
% Data completeness (in resolution range)	88.7 (79.07-2.98) 88.6 (79.07-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.96Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, $R_{free}$	0.208 , 0.288 0.217 , 0.296	Depositor DCC
$R_{free}$ test set	1095 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.2	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	E	0.45	0/41	0.41	0/55
1	F	0.38	0/41	0.67	0/55
2	A	0.46	0/2419	0.68	0/3288
2	B	0.40	0/2419	0.63	0/3288
2	C	0.42	0/2419	0.68	0/3288
2	D	0.42	0/2410	0.64	0/3276
All	All	0.42	0/9749	0.66	0/13250

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	42	0	47	3	0
1	F	42	0	47	7	0
2	A	2366	0	2314	24	0
2	B	2366	0	2314	46	0
2	C	2366	0	2314	41	0
2	D	2357	0	2306	51	0
All	All	9539	0	9342	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.



All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ASN:HB2	2:D:188:ARG:HE	1.43	0.82
2:B:84:ASN:ND2	2:B:180:ASN:ND2	2.28	0.81
2:B:58:LEU:HD13	2:B:82:MET:HB2	1.63	0.81
2:C:40:ARG:HD3	2:C:85:CYS:HA	1.70	0.73
2:C:285:ALA:H	2:D:286:LEU:HD11	1.53	0.73
2:D:51:ASN:CB	2:D:188:ARG:HE	2.02	0.73
2:A:166:GLU:OE2	2:B:1:SER:HB3	1.88	0.72
2:C:213:ILE:HG21	2:C:300:CYS:HB3	1.71	0.71
2:A:188:ARG:HB3	2:A:190:THR:HG22	1.75	0.69
1:E:-1:LEU:HD12	2:B:41:HIS:CG	2.28	0.69
2:D:100:LYS:O	2:D:156:CYS:HA	1.93	0.68
2:A:58:LEU:HD11	2:A:80:HIS:HD2	1.58	0.67
2:B:21:THR:HB	2:B:67:LEU:HB3	1.76	0.67
1:F:-1:LEU:HD12	2:D:41:HIS:CG	2.30	0.65
2:C:109:GLY:HA2	2:C:200:ILE:HD13	1.76	0.65
2:B:84:ASN:ND2	2:B:180:ASN:HD21	1.94	0.65
2:A:87:LEU:HD13	2:A:89:LEU:HD21	1.80	0.63
2:C:163:HIS:HE1	2:C:172:HIS:HB3	1.63	0.62
2:D:45:THR:H	2:D:48:ASP:HB2	1.65	0.61
2:B:243:THR:HG23	2:B:246:HIS:CE1	2.37	0.60
2:B:111:THR:HG22	2:B:129:ALA:HB2	1.83	0.59
2:C:233:VAL:HG21	2:C:269:LYS:HD3	1.85	0.58
2:B:108:PRO:HB2	2:B:132:PRO:HA	1.85	0.58
2:D:40:ARG:HD3	2:D:85:CYS:HA	1.84	0.58
2:B:57:LEU:O	2:B:61:LYS:HG2	2.03	0.58
2:B:84:ASN:HD22	2:B:180:ASN:ND2	2.01	0.58
2:B:9:PRO:HD2	2:B:152:ILE:HD12	1.86	0.57
2:A:113:SER:O	2:A:149:GLY:HA2	2.02	0.57
2:B:36:VAL:HB	2:B:89:LEU:HB2	1.86	0.57
2:C:166:GLU:OE2	2:D:1:SER:HB3	2.05	0.57
2:A:161:TYR:OH	2:A:163:HIS:ND1	2.34	0.57
2:B:40:ARG:HD3	2:B:85:CYS:HA	1.85	0.56
2:C:20:VAL:HG22	2:C:68:VAL:HG22	1.88	0.56
2:D:51:ASN:HB2	2:D:188:ARG:NE	2.19	0.56
1:F:0:GLN:HB3	2:D:142:ASN:HA	1.88	0.56
2:A:111:THR:HG22	2:A:129:ALA:HB2	1.86	0.56
2:C:20:VAL:HG12	2:C:42:VAL:HG21	1.87	0.55
2:D:222:ARG:HE	2:D:222:ARG:H	1.54	0.55
1:F:-1:LEU:HD12	2:D:41:HIS:CD2	2.41	0.55
2:A:44:CYS:HB3	2:A:48:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:-5:THR:HB	2:D:168:PRO:HB3	1.88	0.55
2:C:207:TRP:NE1	2:C:282:LEU:HD12	2.21	0.54
2:B:175:THR:HA	2:B:181:PHE:HA	1.90	0.54
2:A:58:LEU:HD11	2:A:80:HIS:CD2	2.40	0.54
2:B:243:THR:HG23	2:B:246:HIS:ND1	2.23	0.54
1:F:0:GLN:CB	2:D:142:ASN:HA	2.37	0.54
2:C:118:TYR:CE1	2:C:144:SER:HB3	2.43	0.53
2:B:64:HIS:CD2	2:B:65:ASN:ND2	2.77	0.53
2:C:102:LYS:HG2	2:C:104:VAL:HG23	1.91	0.53
2:C:201:THR:HG22	2:C:242:LEU:HD13	1.90	0.53
2:C:70:ALA:HB2	2:C:75:LEU:HD11	1.91	0.52
2:D:186:VAL:H	2:D:192:GLN:NE2	2.07	0.52
2:B:40:ARG:O	2:B:43:ILE:HG12	2.10	0.52
2:D:188:ARG:HB3	2:D:190:THR:HG22	1.91	0.52
2:D:43:ILE:HG22	2:D:66:PHE:HE1	1.75	0.52
2:D:271:LEU:HD11	2:D:281:ILE:HD11	1.91	0.52
2:D:276:MET:HE3	2:D:281:ILE:HG13	1.90	0.52
2:B:14:GLU:HG2	2:B:122:PRO:HG2	1.92	0.52
2:B:85:CYS:HB2	2:B:175:THR:HG21	1.92	0.51
2:B:279:ARG:HH12	2:C:102:LYS:NZ	2.08	0.51
2:D:276:MET:CE	2:D:281:ILE:HG13	2.40	0.51
1:E:-1:LEU:HD12	2:B:41:HIS:CD2	2.45	0.51
2:C:85:CYS:HB2	2:C:175:THR:HG21	1.93	0.51
2:C:10:SER:HB2	2:C:115:LEU:HD13	1.93	0.50
2:D:164:HIS:CD2	2:D:175:THR:HG23	2.48	0.49
2:C:2:GLY:HA3	2:D:139:SER:HA	1.95	0.49
2:C:3:PHE:HE1	2:C:300:CYS:HG	1.59	0.49
2:B:206:ALA:HB2	2:B:293:PRO:HG3	1.95	0.49
2:B:222:ARG:HG2	2:C:107:GLN:HE21	1.77	0.49
2:C:21:THR:HB	2:C:67:LEU:HB2	1.94	0.49
2:A:245:ASP:O	2:A:249:ILE:HG13	2.13	0.49
2:C:100:LYS:HB2	2:C:156:CYS:HA	1.95	0.49
2:D:205:LEU:HD23	2:D:208:LEU:HD12	1.95	0.49
2:D:204:VAL:HG22	2:D:289:ASP:HB3	1.96	0.48
2:D:131:ARG:HG2	2:D:135:THR:O	2.14	0.48
2:D:222:ARG:H	2:D:222:ARG:NE	2.11	0.48
2:C:53:ASN:OD1	2:C:55:GLU:OE1	2.31	0.48
2:D:152:ILE:HG22	2:D:153:ASP:N	2.28	0.48
2:B:44:CYS:HB3	2:B:48:ASP:HB2	1.94	0.48
2:D:205:LEU:O	2:D:208:LEU:HB2	2.13	0.48
2:C:44:CYS:SG	2:C:54:TYR:CE1	3.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:132:PRO:HG2	2:C:198:THR:O	2.14	0.47
2:B:84:ASN:HD21	2:B:180:ASN:HD21	1.62	0.47
2:C:207:TRP:HZ3	2:C:287:LEU:HD23	1.79	0.47
2:B:108:PRO:CB	2:B:132:PRO:HA	2.45	0.47
2:C:106:ILE:HG12	2:C:160:CYS:HB2	1.97	0.47
2:A:95:ASN:HB3	2:A:98:THR:OG1	2.15	0.47
1:F:-5:THR:HB	2:D:168:PRO:CB	2.45	0.47
2:B:167:LEU:HB3	2:B:168:PRO:HD2	1.96	0.46
2:D:111:THR:HG23	2:D:292:THR:HG23	1.97	0.46
2:B:60:ARG:HG3	2:B:61:LYS:HE3	1.98	0.46
2:A:163:HIS:HE1	2:A:172:HIS:HB3	1.80	0.46
2:C:27:LEU:HD13	2:C:39:PRO:HD2	1.96	0.46
2:B:81:SER:HB3	2:B:88:LYS:HB2	1.96	0.46
2:D:138:GLY:O	2:D:172:HIS:HE1	1.98	0.46
2:C:105:ARG:HH11	2:C:176:ASP:HB3	1.81	0.46
2:B:217:ARG:HB3	2:B:220:LEU:HD12	1.98	0.45
2:D:30:LEU:HD22	2:D:148:VAL:HG11	1.98	0.45
2:D:39:PRO:HG2	2:D:145:ALA:HB1	1.97	0.45
2:A:166:GLU:OE1	2:A:172:HIS:NE2	2.43	0.45
2:A:164:HIS:O	2:C:305:PHE:O	2.35	0.45
1:F:-1:LEU:CD1	2:D:41:HIS:CD2	2.99	0.45
2:D:55:GLU:HG3	2:D:82:MET:HE1	1.98	0.45
2:C:3:PHE:CE1	2:C:300:CYS:SG	3.10	0.45
2:A:84:ASN:HB2	2:A:179:GLY:HA3	1.99	0.44
2:C:40:ARG:CD	2:C:85:CYS:HA	2.44	0.44
2:B:210:ALA:HB2	2:B:296:VAL:HG13	1.98	0.44
2:B:270:GLU:OE2	2:B:273:GLN:OE1	2.35	0.44
2:B:163:HIS:HE1	2:B:172:HIS:HB3	1.81	0.44
2:A:163:HIS:CE1	2:A:172:HIS:HB3	2.53	0.44
2:A:91:VAL:HG23	2:A:93:THR:H	1.83	0.44
2:D:17:MET:HG3	2:D:117:CYS:SG	2.58	0.44
2:D:51:ASN:HB2	2:D:188:ARG:HH21	1.82	0.44
2:D:269:LYS:HA	2:D:272:LEU:HD12	1.99	0.44
2:D:249:ILE:HG22	2:D:293:PRO:HG2	1.98	0.44
2:D:53:ASN:HB3	2:D:56:ASP:HB2	2.00	0.43
2:B:198:THR:HA	2:B:238:ASN:OD1	2.18	0.43
2:D:163:HIS:HE1	2:D:172:HIS:HB3	1.83	0.43
2:B:249:ILE:HG22	2:B:293:PRO:HG2	1.99	0.43
2:D:12:LYS:NZ	2:D:99:PRO:HB3	2.33	0.43
2:C:185:PHE:HD1	2:C:192:GLN:HG2	1.84	0.43
2:A:164:HIS:CD2	2:A:175:THR:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:PRO:HD3	2:B:188:ARG:HG3	2.01	0.43
2:D:294:PHE:O	2:D:298:ARG:HB2	2.19	0.43
2:A:8:PHE:HB3	2:A:152:ILE:HD12	2.00	0.42
2:C:234:ALA:O	2:C:239:TYR:HB2	2.19	0.42
2:A:262:LEU:HA	2:A:265:CYS:HB2	2.01	0.42
2:B:84:ASN:ND2	2:B:180:ASN:HD22	2.16	0.42
2:B:95:ASN:HB3	2:B:98:THR:OG1	2.18	0.42
2:C:117:CYS:HA	2:C:122:PRO:HA	2.00	0.42
2:B:165:MET:CE	2:B:185:PHE:HB3	2.50	0.42
2:D:54:TYR:HA	2:D:57:LEU:HD12	2.00	0.42
2:B:31:TRP:CD2	2:B:95:ASN:HB2	2.54	0.42
2:B:279:ARG:NH1	2:C:102:LYS:NZ	2.67	0.42
2:C:101:TYR:O	2:C:156:CYS:SG	2.78	0.42
2:C:111:THR:HG22	2:C:129:ALA:HB2	2.01	0.42
2:D:10:SER:O	2:D:14:GLU:HG3	2.20	0.42
2:C:140:PHE:HB2	2:C:172:HIS:CD2	2.55	0.42
2:A:109:GLY:HA2	2:A:200:ILE:HD13	2.01	0.41
2:C:294:PHE:O	2:C:298:ARG:HB2	2.19	0.41
2:D:188:ARG:HH11	2:D:190:THR:HB	1.85	0.41
2:B:209:TYR:HB3	2:B:253:LEU:HD22	2.03	0.41
2:B:140:PHE:HB3	2:B:144:SER:OG	2.20	0.41
2:D:299:GLN:HE21	2:D:299:GLN:HB2	1.64	0.41
2:D:27:LEU:HD13	2:D:39:PRO:HD2	2.02	0.41
2:A:167:LEU:HB3	2:A:168:PRO:HD2	2.03	0.41
2:C:52:PRO:HD3	2:C:188:ARG:HG3	2.02	0.41
2:D:186:VAL:H	2:D:192:GLN:HE22	1.67	0.41
2:A:27:LEU:HB2	2:A:145:ALA:O	2.21	0.41
1:E:-1:LEU:HD23	2:B:189:GLN:HG3	2.03	0.41
2:A:216:ASP:O	2:A:217:ARG:HG3	2.21	0.41
2:D:161:TYR:CE1	2:D:174:GLY:HA3	2.55	0.41
2:B:233:VAL:HG21	2:B:269:LYS:HD3	2.03	0.40
2:D:47:GLU:HG2	2:D:50:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	4/6 (67%)	4 (100%)	0	0	100	100
1	F	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
2	A	304/306 (99%)	280 (92%)	19 (6%)	5 (2%)	9	38
2	B	304/306 (99%)	274 (90%)	26 (9%)	4 (1%)	12	43
2	C	304/306 (99%)	265 (87%)	36 (12%)	3 (1%)	15	50
2	D	303/306 (99%)	264 (87%)	38 (12%)	1 (0%)	41	74
All	All	1223/1236 (99%)	1090 (89%)	120 (10%)	13 (1%)	14	47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	154	TYR
2	B	47	GLU
2	C	154	TYR
2	B	63	ASN
2	A	155	ASP
2	B	43	ILE
2	C	283	GLY
2	A	50	LEU
2	C	134	PHE
2	D	240	GLU
2	A	2	GLY
2	A	11	GLY
2	B	52	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	5/5 (100%)	4 (80%)	1 (20%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	5/5 (100%)	4 (80%)	1 (20%)	1	6
2	A	262/262 (100%)	242 (92%)	20 (8%)	13	41
2	B	262/262 (100%)	245 (94%)	17 (6%)	17	48
2	C	262/262 (100%)	234 (89%)	28 (11%)	6	24
2	D	261/262 (100%)	230 (88%)	31 (12%)	5	21
All	All	1057/1058 (100%)	959 (91%)	98 (9%)	9	31

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	0	GLN
2	A	1	SER
2	A	4	ARG
2	A	5	LYS
2	A	25	THR
2	A	44	CYS
2	A	45	THR
2	A	48	ASP
2	A	55	GLU
2	A	87	LEU
2	A	102	LYS
2	A	155	ASP
2	A	169	THR
2	A	188	ARG
2	A	190	THR
2	A	192	GLN
2	A	197	ASP
2	A	227	LEU
2	A	256	GLN
2	A	288	GLU
2	A	299	GLN
2	B	12	LYS
2	B	47	GLU
2	B	49	MET
2	B	58	LEU
2	B	67	LEU
2	B	69	GLN
2	B	73	VAL
2	B	74	GLN
2	B	87	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	107	GLN
2	B	110	GLN
2	B	128	CYS
2	B	154	TYR
2	B	216	ASP
2	B	224	THR
2	B	227	LEU
2	B	228	ASN
1	F	0	GLN
2	C	1	SER
2	C	3	PHE
2	C	4	ARG
2	C	16	CYS
2	C	19	GLN
2	C	22	CYS
2	C	48	ASP
2	C	58	LEU
2	C	60	ARG
2	C	62	SER
2	C	64	HIS
2	C	80	HIS
2	C	84	ASN
2	C	87	LEU
2	C	89	LEU
2	C	106	ILE
2	C	110	GLN
2	C	114	VAL
2	C	128	CYS
2	C	192	GLN
2	C	217	ARG
2	C	248	ASP
2	C	269	LYS
2	C	280	THR
2	C	286	LEU
2	C	289	ASP
2	C	291	PHE
2	C	292	THR
2	D	6	MET
2	D	10	SER
2	D	48	ASP
2	D	56	ASP
2	D	78	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	87	LEU
2	D	107	GLN
2	D	121	SER
2	D	128	CYS
2	D	142	ASN
2	D	158	SER
2	D	165	MET
2	D	181	PHE
2	D	186	VAL
2	D	200	ILE
2	D	216	ASP
2	D	222	ARG
2	D	223	PHE
2	D	224	THR
2	D	225	THR
2	D	227	LEU
2	D	233	VAL
2	D	242	LEU
2	D	243	THR
2	D	245	ASP
2	D	248	ASP
2	D	263	ASP
2	D	271	LEU
2	D	284	SER
2	D	286	LEU
2	D	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	A	256	GLN
2	B	64	HIS
2	B	84	ASN
2	B	180	ASN
2	B	256	GLN
1	F	0	GLN
2	C	64	HIS
2	C	80	HIS
2	C	214	ASN
2	D	41	HIS
2	D	192	GLN
2	D	299	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	6/6 (100%)	0.44	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	81, 82, 83, 83	0
1	F	6/6 (100%)	0.94	1 (16%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	74, 78, 84, 85	0
2	A	306/306 (100%)	-0.11	2 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">74</span>	30, 48, 67, 79	0
2	B	306/306 (100%)	-0.02	4 (1%) <span style="border: 1px solid blue; padding: 2px;">77</span> <span style="border: 1px solid blue; padding: 2px;">59</span>	33, 59, 88, 99	0
2	C	306/306 (100%)	0.34	11 (3%) <span style="border: 1px solid red; padding: 2px;">42</span> <span style="border: 1px solid red; padding: 2px;">26</span>	45, 71, 92, 103	0
2	D	305/306 (99%)	0.21	9 (2%) <span style="border: 1px solid gray; padding: 2px;">50</span> <span style="border: 1px solid red; padding: 2px;">31</span>	41, 65, 94, 108	0
All	All	1235/1236 (99%)	0.11	27 (2%) <span style="border: 1px solid blue; padding: 2px;">62</span> <span style="border: 1px solid red; padding: 2px;">42</span>	30, 61, 90, 108	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	266	ALA	4.5
2	A	155	ASP	4.0
2	D	237	TYR	3.9
2	C	224	THR	3.7
2	D	154	TYR	3.6
2	D	242	LEU	3.3
1	F	-1	LEU	3.2
2	D	285	ALA	3.0
2	D	188	ARG	3.0
2	C	281	ILE	2.8
2	C	287	LEU	2.8
2	C	294	PHE	2.6
2	D	201	THR	2.6
2	D	73	VAL	2.5
2	B	59	ILE	2.5
2	D	241	PRO	2.5
2	D	50	LEU	2.5
2	C	152	ILE	2.5
2	B	66	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	306	GLN	2.4
2	C	219	PHE	2.4
2	B	256	GLN	2.4
2	C	268	LEU	2.3
2	A	69	GLN	2.3
2	C	50	LEU	2.2
2	C	31	TRP	2.2
2	C	39	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.